REPORT DOCUMENTATION PAGE

2. REPORT DATE

Public reporting burden for this collection of information is estimated to average 1 hour per response, including athering and maintaining the data needed, and completing and reviewing the collection of information. Send collection of information, including suggestions for reducing this burden, to Washington Headquarters Services Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork R

1. AGENCY USE ONLY (Leave

AFRL-SR-BL-TR-98-

3. REPORT TYPE AND DATES COVERED

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	Blank)	20 Jan 1998	Final	01 Dec 1994	30 Nov 1997	
4.	TITLE AND SUBTITLE Numerical Modeling and Analysis of Transient Electromagnetic Wave Interaction with Dispersive Targets			5. FUNDING NUMBERS F49620-95-1-0014		
6.	. AUTHORS Peter G. Petropoulos					
7.	PERFORMING ORGANIZATION NA Southern Methodist University Department of Mathematics P O Box 750156 Dallas, TX 75275-0156				8. PERFORMING ORGANIZATION REPORT NUMBER 5-25169	
9.	SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) AFOSR/PKA 110 Duncan Avenue Room B115 Bolling AFB DC 20332-8080					
11	11. SUPPLEMENTARY NOTES Research results published in the Journals: Josa-A, Aces Journal, IEEE-AP Transactions, Journal of Computational Physics					
12	12a. DISTRIBUTION / AVAILABILITY STATEMENT Available to the public				12b. DISTRIBUTION CODE	
13	Analytical and numerical techniques were developed for modeling transient electromagnetic wave propagation in dispersive dielectrics. Time-domain asymptotic techniques were used to understand the decay of pulses in such media and to develop energy estimates useful in RFR dosimetry. Fourth-order accurate numerical schemes were proposed for such problems and analyzed. Due to the large stencil of these schemes special absorbing boundary conditions were developed and analyzed. Numerical tests indicated a four orders of magnitude superiority of our conditions over the classical techniques.					
					19980223 154	

14. SUBJECT TERMS 15. NUMBER OF PAGES Dispersive Dielectrics, Absorbing Boundary Conditions, Finite Difference Schemes, 7 **Asymptotic Methods** 16. PRICE CODE 18. SECURITY CLASSIFICATION 17. SECURITY CLASSIFICATION 19. SECURITY CLASSIFICATION 20. LIMITATION OF ABSTRACT OF REPORT OF THIS PAGE OF ABSTRACT UL Unclassified Unclassified Unclassified

NSN 7540-01-280-5500

Numerical Modeling and Analysis of Transient Electromagnetic Wave Interaction with Dispersive Targets

Peter G. Petropoulos Department of Mathematics Southern Methodist University Dallas, TX 75275

20 January 1998

Final Report for Period 1 December 1994 - 30 November 1997 (Grant F49620-95-1-0014)

Prepared for AIR FORCE OFFICE OF SCIENTIFIC RESEARCH/NM 110 Duncan Avenue, Suite B115 Bolling AFB, DC 20332-0001

1 Technical Summary of Research Accomplished

The citations in this Section refer to the papers in the References.

We examined [1] electromagnetic pulse propagation in anomalously dispersive media, using the Debye model as an example. Short-pulse, long-pulse, short-time, and long-time approximations and amplitude rate-of-decay estimates were derived with asymptotic methods. We also studied the following problem: Knowing only the peak amplitude and energy density of an incident pulse, what can be said about the amplitude of the propagated pulse? We provided tight upper and lower bounds for the propagated amplitude, which may be useful in controlling the electromagnetic interference or the damage produced in dispersive media. We explained a factor-of-nine effect in the speed of pulses in a Debye model for water, which seems to have been previously unnoticed, and we also explained some observations from experimental studies of pulse propagation in biological materials which were presented in W. D. Hurt, "Measurement of specific absorption rate in human phantoms exposed to simulated Air Force radar emissions," USAFSAM-TR-84-16 (June 1984) Armstrong Laboratory, Brooks AFB, TX, 1984. Finally, we proposed some guidelines for sample size in Transmission Time Domain Spectroscopy studies of dielectrics described in B. Gestblom and E. Noreland, "Transmission Methods in Dielectric Time Domain Spectroscopy," J. Phys. Chem., v. 81, 782-788 (1977).

In [2] we addressed the numerical solution of the equations describing electromagnetic pulse propagation in geometrically complex Debye-dispersive dielectrics that are used in the development of safety standards for human exposure to non-ionizing radiation. Such dielectric models are described in W. D. Hurt, "Multiterm Debye dispersion relations for permittivity of muscle," IEEE Trans. Biomed. Engnr., v. BME-32, 60-64 (1985). Debye dispersion is a relaxation process, a phenomenon which occurs when the underlying material is forced into non-equilibrium due to the passing waves. This relaxation is typically stiff in applications, and the system of equations is then singularly perturbed. Such systems are notoriously expensive to solve with standard numerical methods. We reviewed previous work related to the numerical solution of such problems, and considered a representative numerical scheme in order to elucidate the nature of the challenge posed to Computational Electromagnetics by the stiffness. Further, an analysis of the stiffness via the method of matched asymptotic expansions allowed us to elucidate the wave behavior inside such dielectrics and to propose a scheme that seemed "natural" for the problem at hand. Then, quidelines were developed for correctly setting the discretization when solving such problems with numerical methods. Significantly, the identification of two speeds in such dielectrics is central to these guidelines; the smaller of the two speeds must be used to set the spatial cell size, while the larger, along with the determined spatial cell size, must be used in the Courant stability condition to set the timestep for the simulation. For schemes that discretize time to the same accuracy as space, this guideline indicates that the discretization requirements quickly lead realistic problems out of reach of existing computational resources when high accuracy is required.

To determine whether one could employ alternative time integration schemes in order to avoid having to resolve the stiffness in lossy/dispersive media we studied discretizations of the equations describing transient propagation in a model dielectric. In [3] we first determined the stability condition and then analyzed the accuracy of the exponential and centered time-differencing schemes for FD-TD in an isotropic, homogeneous, lossy dielectric with electric and magnetic conductivities, σ and σ^* respectively. We showed that these schemes are equivalent and determined that for accuracy both schemes must be used with a timestep that finely resolves the electric and magnetic conduction current relaxation timescales. In addition, the implications of these results for PML-type absorbing boundary conditions, which employ such media, were discussed.

Our work in [2] identified "natural" schemes for modeling propagation and scattering in dispersive dielectrics. These schemes are second-order accurate in time and fourth-order accurate in space and allow for decoupling the timestep and spatial cell size. By this decoupling we mean that they allow for the spatial cell size to be set independently of the timestep as long as the relevant stability condition is satisfied. Thus, in a dispersive medium one would set the spatial cell size as described in [2] to resolve the small length scale introduced by the slow speed, and the timestep as described in [3] to resolve the time stiffness. In this way, the timestep does not result in an unnecessarily small spatial step which will make the simulation expensive in terms of storage. The longer spatial stencil of these high-order schemes requires appropriate absorbing boundary conditions to truncate the computational sapce over which typical scattering problems involving dispersive targets are to be solved. Up to the completion of our work there have not been any satisfactory absorbing boundary procedures for high-order stencils in the literature. We addressed this problem in [4] by developing, implementing, and demonstrating a reflectionless sponge layer for truncating computational domains in which the time-dependent Maxwell equations are discretized with high-order staggered non-dissipative finite difference schemes. The well-posedness of the Cauchy problem for the sponge layer equations was proved, and the stability and accuracy of their discretization was analyzed. With numerical experiments we compared our approach to classical techniques for domain truncation that are based on second- and third-order physically-accurate local approximations of the true radiation condition. These experiments indicated that our sponge layer offers a greater than three order of magnitude reduction of the lattice truncation error over that afforded by the classical techniques. We also showed that our strongly well-posed sponge layer performed as well as the ill-posed split-field Berenger PML absorbing boundary condition, and that, being an unsplit-field approach, our sponge layer achieves a $\sim 25\%$ savings in computational effort over that required by a split-field approach.

The results of [4] were very encouraging, particularly after extensive numerical runs which indicated that the reduction of the error due to domain truncation with a sponge layer can be driven > 4 orders of magnitude below the error achieved by the classical techniques. In light of many scattering problems that are better posed in cylindrical and spherical coordinates we developed in [5] reflectionless sponge layers for the numerical solution of the frequency- and time-domain Maxwell equations in cylindrical, and spherical coordinates. Our approach, in contrast to those of F. Collino and P. Monk, "The Perfectly Matched Layer in Curvilinear Coordinates," SIAM J. Scientific Computing, to appear, 1997 & F. L. Teixeira and W. C. Chew, "Perfectly Matched Layer in Cylindrical Coordinates," 1997 IEEE Antennas and Propagation Society International Symposium Proceedings, vol. 3, pp. 1908-1911, does not require an arbitrary splitting of the fields to obtain the time-domain formulation. We proved the resulting time-domain equations form causal, strongly well-posed hyperbolic systems in the two curvilinear coordinate systems, and representative numerical simulations demonstrated that such layers result, as expected, in ≥ 4 orders of magnitude less reflected energy than that obtained with classical approaches. Also, when discretized with a popular 2nd-order staggered leapfrog scheme, mesh refinement showed the reflectionless property of the layer converges $O(h^2)$, i.e., to the order of accuracy of the interior scheme, where h is the spatial mesh size. Our sponge layer does not require additional spatial derivatives in its implementation hence it will always converge at the rate of the spatial discretization used to solve Maxwell's equations over the computational domain.

2 Invited Conference Papers

"Fourth-Order Accurate Staggered Finite Difference Schemes for the Time-Dependent Maxwell Equations," Invited Paper in the Proceedings of the 13th Dundee Conference on Ordinary and Partial Differential Equations Volume V, Pitman Research Notes in Mathematics Series, #370, pp. 85-107, UK, 1997.

"The Application of PML ABCs in High-Order FD-TD Schemes," 13th Annual Review of Progress in Applied Computational Electromagnetics Proceedings, v. 2, pp. 884-891, Monterey, CA, March 1997. Invited Paper in Special Session Titled "PML: Theoretical and Numerical Implementation Issues," Co-organized with A.C. Cangellaris (UIUC).

"High-Order Nondissipative Staggered Schemes for Maxwell's Equations," *IEEE-APS International Symposium Proceedings*, vol. 1, pp. 114-117, Montreal, Canada, July 1997. Invited Paper in APS Special Session Titled "Interdisciplinary Computational Electromagnetics,"

Organized by J. S. Shang (WPAFB).

3 Invited and Contributed Presentations

"Computation of Scattering by Dielectrics Exhibiting Disparate Length and Time Scales," USAF Electromagnetics Workshop, Brooks AFB, January 1995.

"The Numerical Computation of Singularly Perturbed Linear Dispersive Waves," *UT-Austin Symposium on Advances and Trends in Computational and Applied Mathematics*, Austin TX, April 1995.

"Finite Difference Schemes for the Long-time Solution of the Maxwell Equations in Nonlinear Dielectrics with Dispersion and Absorption," Invited Mini-symposium (Pulse Dynamics in Novel Nonlinear Optical Systems) Presentation at the Third SIAM Conference on Applications of Dynamical Systems, Snowbird UT, May 1995.

"High-Order Finite Difference Schemes for the Time Dependent Maxwell's Equations in Materials with Memory," *Invited Presentation at the First ICASE Computational Electromagnetics Workshop*, NASA Langley, VA, June 1995.

"Computing Dispersive Waves," *Invited Seminar Presentation*, Department of Mathematics, New Jersey Institute of Technology, Newark NJ, October 1995.

"The Comparative Cost, and Order of Accuracy on Dielectric Interfaces, for Second- and Fourth-Order Accurate Staggered Grid Methods for Maxwell's Equations," *USAF Electromagnetics Workshop*, Brooks AFB, January 1996.

"Fourth-Order Accurate Staggered Finite Difference Schemes for the Time-Dependent Maxwell Equations," Invited Plenary Talk at the 13th Dundee Conference on Ordinary and Partial Differential Equations, University of Dundee, Scotland, June 1996.

"Reflectionless ABCs for High-Order Staggered Schemes," USAF Electromagnetics Workshop, Brooks AFB, January 1997.

"The Application of PML ABCs in High-Order FD-TD Schemes," 13th Annual Review of Progress in Applied Computational Electromagnetics, Monterey, CA, March 1997. Invited Presentation in Special Session Co-organized with A.C. Cangellaris (UIUC).

"High-Order Nondissipative Staggered Schemes for Maxwell's Equations," *IEEE-APS International Symposium*, Montreal, Canada, July 1997. Invited Presentation in Special Session Titled "Interdisciplinary Computational Electromagnetics," Organized by J. S. Shang (WPAFB).

Invited Lecturer at the NATO Advanced Summer Institute on CEM (July-August 1997, Samos, Greece). Titles of the Three Lectures Delivered:

- a) Fundamentals of the FD-TD method.
- b) High-Order and Compact Finite-Difference Schemes for CEM.
- c) FD-TD Simulation of Wave Propagation in Dispersive Media.

"Perfectly Matched Sponge Layers as ABCs for the Numerical Solution of Maxwell's Equations in Rectangular, Cylindrical, and Spherical Coordinates," *Invited Presentation at the Waves, Applied Math, Inverse problems and Electromagnetic Scattering Seminar*, Department of Mathematics, University of Delaware, Newark DE, November 1997.

4 Consultative And Advisory Functions To Other Laboratories And Agencies

Throughout the period covered by this report I had extensive interactions of a consultative/advisory nature with Dr. T.M. Roberts (Rome Laboratory/ERAA, Hanscom AFB). The topics of these interactions were finite difference solvers for the time-domain Maxwell equations, and apply-and-forget absorbing boundary conditions for the finite difference solution of scattering problems of common interest.

5 Transitions

Several finite difference codes, each implementing different absorbing boundary procedures were transitioned to T.M. Roberts (Rome Laboratory/ERAA, Hanscom AFB) as aids in his USAF-sponsored research. One of the absorbing boundary conditions implemented, along with the instructions on its correct use, were direct results of the present grant.

Similar codes, and some other codes (an integral equation solver, and a code implementing an exact solution of a model scattering problem) were similarly transitioned to the group of Prof. D. Gottlieb (Brown U.) enabling the relevant USAF-sponsored research to produce new results in a short time.

References

- [1] T. M. Roberts and P. G. Petropoulos, "Asymptotics and Energy Estimates for Electromagnetic Pulses in Dispersive Media," J. Opt. Soc. Am. A, vol. 13, no. 6, pp. 1204-1217, 1996.
- [2] P. G. Petropoulos, "The Computation of Linear Dispersive Electromagnetic Waves," *ACES Journal*, vol. 11, pp. 8-16, Jan. 1996.
- [3] P. G. Petropoulos, "Analysis of Exponential Time-Differencing for FD-TD in Lossy Dielectrics," *IEEE Trans. on Antennas and Propagation*, vol. 45, no. 6, pp. 1054-1057, 1997.
- [4] P. G. Petropoulos, L. Zhao and A. C. Cangellaris, "A Reflectionless Sponge Layer Absorbing Boundary Condition for the Solution of Maxwell's Equations with High-Order Staggered Finite Difference Schemes," J. Computational Physics, accepted, to appear 1998.
- [5] P. G. Petropoulos, "Unsplit Perfectly Matched Layer Absorbing Boundary Conditions for the Numerical Solution of Maxwell's Equations in Rectangular, Cylindrical and Spherical Coordinates," *IEEE Transactions on Antennas and Propagation*, in review, 1997.